DISCOVERING NOVEL GAS-PHASE NITROGEN-HETEROCYCLE FORMATION PATHWAYS WITH AN AB INITIO NANOREACTOR

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Nitrogen-containing heterocycles pose an intriguing astrochemical mystery. 45 different varieties have been detected on meteorites with non-terrestrial isotopic abundances, but none have been detected in space, despite numerous search attempts. It is unclear if these species are more likely to form through low-temperature gas-phase chemistry, photoprocessing of icy grains, aqueous chemistry in a meteorite parent body, or a combination of processes. Further exploration of this question requires a broader catalog of potential N-heterocycle precursors, particularly for low temperature gas-phase chemistry. Here, results of *ab initio* molecular dynamics simulations of gas-phase N-heterocycle forming reactions will be discussed. These simulations were performed with an *ab initio* nanoreactor, a computational tool developed for chemical reaction discovery. Multiple novel gas-phase N-heterocycle formation pathways have been revealed, and many reactants are similar to known interstellar molecules. These simulations also reinforce previous experimental and theoretical studies which demonstrated that smaller N-heterocycles are potential precursors to larger ones. While these simulations cannot provide direct insight into interstellar chemistry, they have revealed nonintuitive N-heterocycle precursors that warrant further experimental and astronomical study.